

National Aeronautics and Space Administration



# Project Status Report

## High End Computing Capability Strategic Capabilities Assets Program

10 July 2012

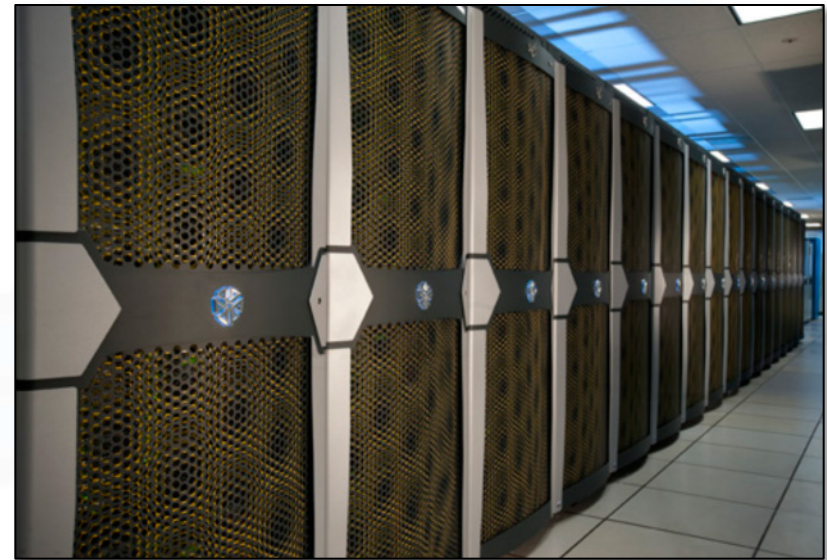
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# Pleiades Sustained Performance Rises to 1.24 Petaflops on the LINPACK Benchmark



- Following the installation of 24 SGI ICE X “Sandy Bridge” racks in May, a team of HECC, SGI, and Mellanox engineers achieved a sustained performance of 1.243 petaflops (PF) using the LINPACK benchmark on Pleiades.
- This measurement ranks Pleiades as the 11<sup>th</sup> fastest supercomputer on the June 2012 TOP500 list, and places the system as the 4<sup>th</sup> fastest supercomputer in the United States.
- In addition, Pleiades ranks as the 8<sup>th</sup> fastest supercomputer on the TOP500 list that does not utilize graphics processors to accelerate computation.
- Using four different generations of processors and three different generations of InfiniBand on Pleiades, the expansion increased the sustained performance rate of LINPACK by 14%, and achieved 71.3% of the theoretical peak performance.

**Mission Impact:** Through the HECC Project, NASA science and engineering users can make highly efficient use of their computing time on Pleiades, one of the top computational resources in the world.



**Figure:** Pleiades now delivers a sustained performance rate of 1.24 petaflops (PF) to support more than 1,200 users across the country who rely on the system to perform their large, complex calculations.

**POCs:** Bob Ciotti, [bob.ciotti@nasa.gov](mailto:bob.ciotti@nasa.gov), (650) 604-4408,  
NASA Advanced Supercomputing Division;  
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NASA Advanced Supercomputing Division, Computer Sciences Corp.

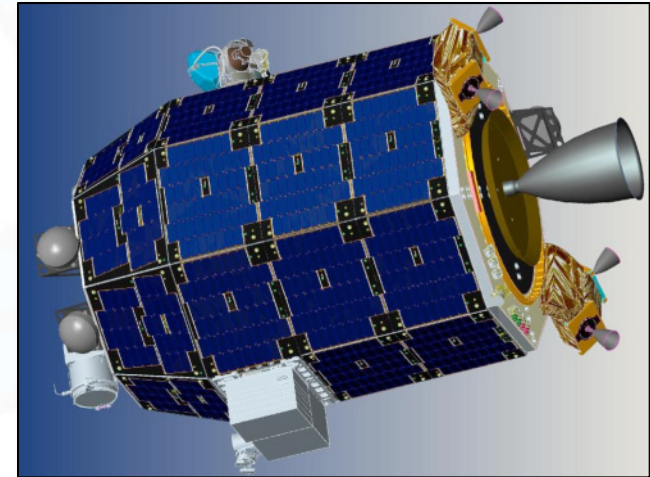


# Optimization Support Improves NASA Kennedy Code Performance 1000-Fold



- HECC optimization experts have obtained a 1000x performance improvement in a code that calculates trajectories of lunar dust, soil, and gravel blown by the exhaust plume of a lunar lander.
- Researchers at NASA Kennedy's Granular Mechanics and Regolith Operations Lab plan to use the code as part of an effort to protect Apollo "heritage sites" from Google's Lunar X-Prize landers, and for analyzing data from NASA's upcoming LADEE mission in 2013.
- HECC staff employed a kdtree-based point location strategy for the code's unstructured grid flow data, and an error-monitoring adaptive stepper for the trajectory integrator.
- KSC has requested HECC assistance with their envisioned next step: coupling the particle integrator with a hybrid code for calculating concurrent exhaust/dust interactions along a lander descent path.

**Mission Impact:** Optimizing the NASA Kennedy code allows researchers to obtain their results and reach their milestones on time, while utilizing greatly reduced compute resources for their tasks than originally anticipated.



**Figure:** A computer-generated model of the LADEE spacecraft. The mission team is interested in observing dust ejected by a Google Lunar X-Prize lander to measure the perturbations to the natural lunar environment. Predictions from NASA Kennedy exhaust plume models can be compared with LADEE measurements, which will in turn help calibrate the models. Image: NASA/Ames

**POC:** Chris Henze, [chris.henze@nasa.gov](mailto:chris.henze@nasa.gov), (650) 604-3959, NASA Advanced Supercomputing Division

# HECC Enhances Pleiades Stability and Usability



- HECC system engineers corrected several issues with InfiniBand, Lustre and the MPI library on Pleiades to enhance the stability and usability of the system.
- HECC application engineers discovered a problem with the latest release of the SGI's MPI implementation that would cause some jobs to fail. After extensive debugging and working with SGI support, the team was able to narrow down the issue for SGI engineering to resolve.
- After the recent Lustre upgrade, several bugs were uncovered that were not found during testing. HECC system engineers working with Whamcloud(a Lustre support vendor) were able to quickly provide patches to seven bugs that involved updating both the client nodes and the servers.
- Additional refinements to the InfiniBand FDR firmware made by Mellanox were tested by SGI and HECC system engineers. This new firmware showed improvements in the stability of the InfiniBand links and results in fewer system errors for HECC users.

**Mission Impact:** The skill set of the HECC staff across a broad spectrum of technical areas enables timely resolution of complex system problems. The time from initial deployment to full utilization of new assets is greatly reduced by cooperation between HECC and the vendor community.



**Figure:** The Pleiades computer system is one of the most complex systems in the world with four generations of processors, three generations of InfiniBand network technologies and a complex parallel file system

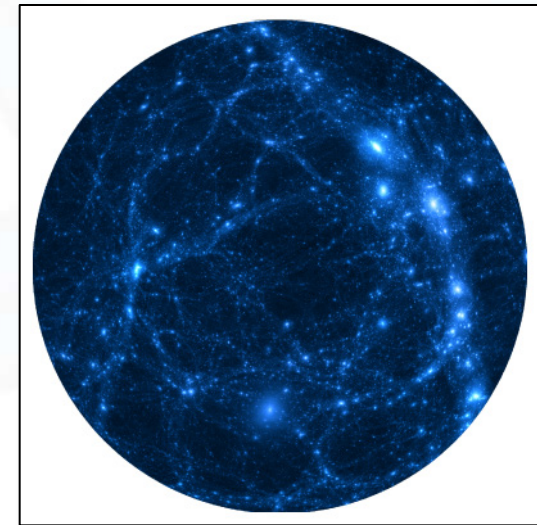
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Davin Chan, [davin.s.chan@nasa.gov](mailto:davin.s.chan@nasa.gov), (650) 604-3613, NASA Advanced Supercomputing Division, Computer Sciences Corp.

# HECC Supports Simulations, Visualization of Cosmology and Galaxy Formation



- Researchers at the University of California, Santa Cruz (UCSC) and New Mexico State University are using cosmological simulations to understand how galaxies formed within the Lambda Cold Dark Matter ( $\Lambda$ CDM) universe.
- The Bolshoi simulations, available to astronomers worldwide, model the evolution of the large-scale structure of the universe with unprecedented accuracy.
- UCSC's hydrodynamic simulations of galaxies forming in the standard  $\Lambda$ CDM framework provide theoretical support for interpretation of data from the Hubble Space Telescope and other observatories.
- Pleiades and Columbia enable researchers to run these high-resolution simulations, and collaboration with HECC visualization experts is crucial for viewing, interpreting, and presenting results.

**Mission Impact:** For the first time, the science community has accurate models of the large-scale structures of the universe – enabled by both HECC's powerful supercomputers and its data analysis and visualization expertise.



**Figure:** This image from the Constrained Local Universe Simulations (CLUES), shown here in “dome view,” was featured as the opening segment of the inaugural show at the Chicago Adler Planetarium’s 8,000-by-8,000-pixel dome in July 2011. Stephan Gottloeber, Astrophysics Institute Potsdam; Chris Henze, NASA/Ames.

*\*HECC provided supercomputing resources and services in support of this work.*

**POC:** Joel Primack, [joel@ucsc.edu](mailto:joel@ucsc.edu), (831) 459-2580, University of California, Santa Cruz/UC-High-Performance AstroComputing Center



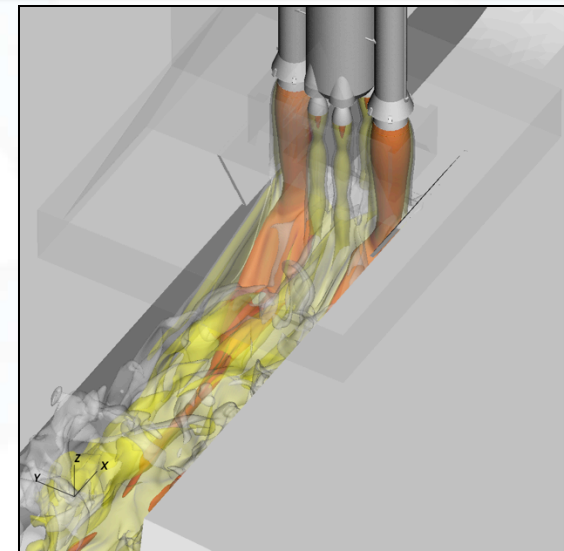
# Extensive CFD Simulations Support Development of 21<sup>st</sup> Century Launch Complex



- Modeling and simulation experts at NASA Ames used Pleiades to perform computational fluid dynamics (CFD) simulations of launch environment conditions for development of the Agency's 21<sup>st</sup> Century Launch Complex at KSC.
- Using ultra-large-scale CFD simulations, the team modeled the entire launch vehicle, platform, and flame trench configurations and computed the complex plume physics involved during ignition and liftoff.
- Each case required 100-150 thousand processor-hours on Pleiades – a total of ~4 million hours for the 4-month project.
- These analyses will help ensure that the new launch complex can handle the significantly higher thrusts of the heavy-lift Space Launch System and other new vehicles.

*\*HECC provided supercomputing resources and services in support of this work.*

**Mission Impact:** CFD launch environment simulations assess plume conditions during ignition and liftoff to ensure that new launch pad designs can safely accommodate next-generation launch vehicles.



**Figure:** Visualization from a CFD simulation of plume containment for the design of NASA's 21st Century Launch Complex. The image shows the ignition plume from a potential Space Launch System vehicle at full thrust as it flows into the flame trench below the launch pad. Simulations such as these support redesign of the flame trench main deflectors for the new launch complex. Michael Barad, Shayan Moini-Yetka, NASA/Ames.

**POC:** Cetin Kiris, [cetin.c.kiris@nasa.gov](mailto:cetin.c.kiris@nasa.gov), (650) 604-4485,  
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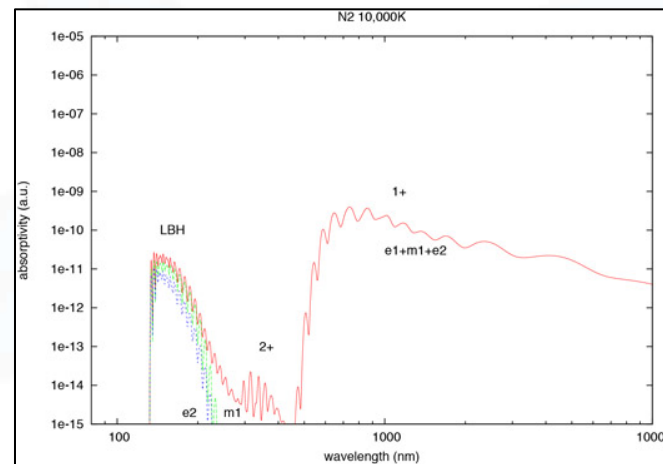
# Quantum Chemistry Calculations for Ultra-Violet Spectra of Air Molecules



- Development of the heat shield for spacecraft entering Earth's atmosphere requires accurate spectra of air molecules at temperatures up to 10,000 Kelvin for lunar return.
- A NASA Ames researcher is carrying out extensive quantum chemistry calculations for key air molecules, covering each possible spin and space symmetry.
- The spectra generated by these quantum chemistry computations are being used with NASA's Ames radiative code, HyperRad, to reduce the uncertainty in heating predictions for spacecraft.
- The enormous number of complex calculations required for this work could not have been carried out without the large number of processors available on the Pleiades supercomputer.

*\*HECC provided supercomputing resources and services in support of this work.*

**Mission Impact:** HECC resources are enabling more accurate predictions for heatshield designs to improve the probability of mission success and enable vehicle payloads to be maximized, as well as to influence the design and planning of all future missions involving atmospheric reentry.



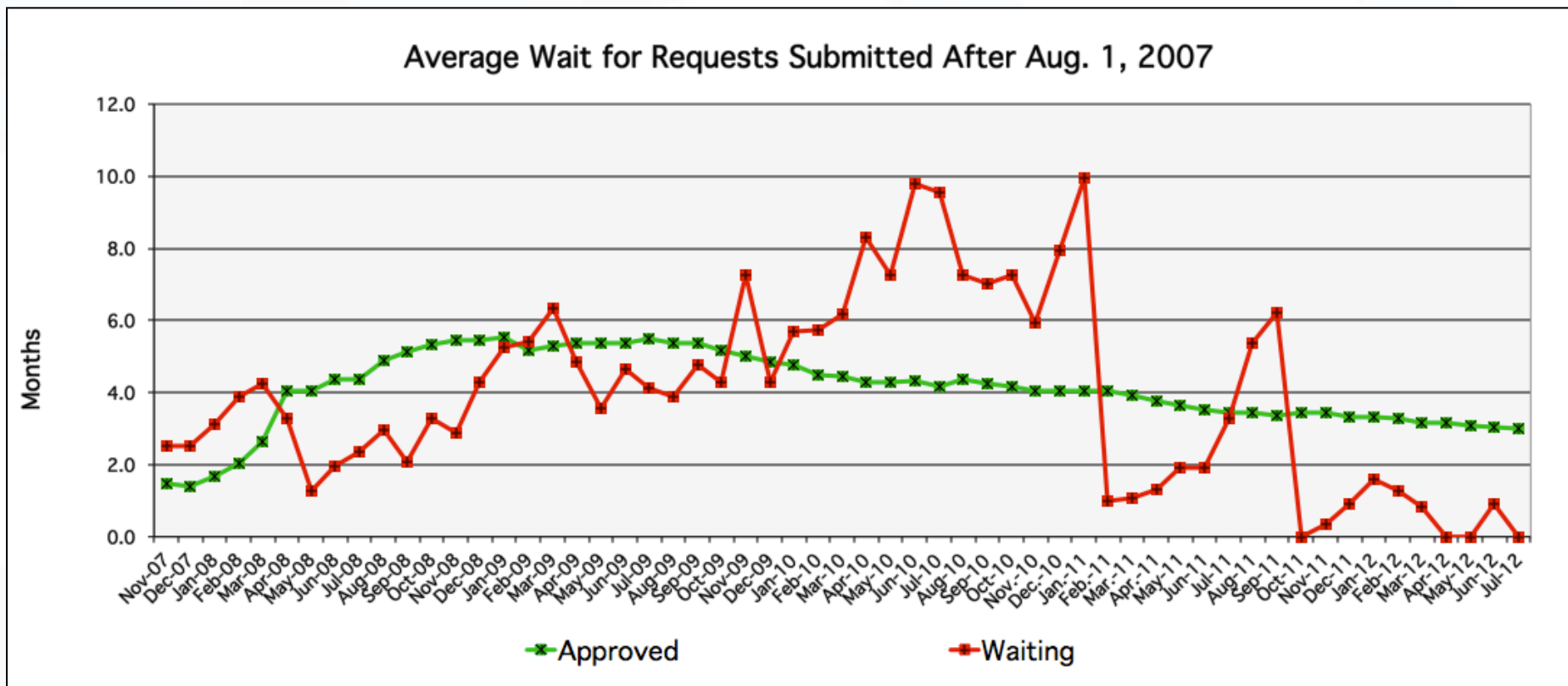
**Figure:** Absorptivity of N<sub>2</sub> at 10,000 Kelvin, from current calculations.  
David Schwenke, NASA/Ames

**POC:** David Schwenke, [david.w.schwenke@nasa.gov](mailto:david.w.schwenke@nasa.gov), (650) 604-6634,  
NASA Advanced Supercomputing Division

# Status of Requests for NAS Computer Accounts by non-U.S. Citizens



- Requests approved: 9; New requests received: 0; Requests waiting: 0.
- The time to approval continues to improve.





# HECC Facility Hosts Several Visitors and Tours in June 2012



- HECC hosted 6 tour groups in June; guests learned about the Agency-wide missions being supported by Pleiades, and viewed scientific results on the hyperwall. Visitors included:
  - As part of a Science, Technology, Engineering and Mathematics (STEM) camp, 36 students (8-12 years old) and 4 teachers from the Bay Area's Greene Scholars Program were given a tour and hyperwall demo – the students were enthusiastic and appreciative.
  - 30 members of the California Biodiversity Council, including representatives from several state agencies focused on California's biodiversity; the group is interested in Ames' Earth science research and the applications to biodiversity issues in California.
  - Media representatives from the "Science/Engineering Journalism Boot Camp on Computational Astronomy: From Planets to Cosmos," hosted by the University of California, Santa Cruz; the group received a non-technical review of science being performed on Pleiades.



**Figure:** Visualization expert Chris Henze interacts with an enthusiastic group of young STEM students during a tour of the Pleiades supercomputer.

**POC:** Gina Morello, [gina.f.morello@nasa.gov](mailto:gina.f.morello@nasa.gov), (650) 604-4462,  
NASA Advanced Supercomputing Division

# Presentations and Papers



- **“Magneto-Convection,”** Robert Stein, Philosophical Transactions of The Royal Society, July 13, 2012, vol. 370 no. 1970.\*  
<http://rsta.royalsocietypublishing.org/content/370/1970/3070.short>
- **“On the Formation of Active Regions,”** Robert Stein and Ake Nordlund, The Astrophysics Journal, Volume 753, Number 1, June 14, 2012.\*  
<http://iopscience.iop.org/2041-8205/753/1/L13>
- **“The Impact of High-End Computing on NASA Missions,”** R. Biswas, J. Dunbar, J. Hardman, F. R. Bailey, L. Wheeler, S. Rogers, IT Professional, Volume 14, Issue 2, March-April 2012.  
[http://ieeexplore.ieee.org/xpls/abs\\_all.jsp?arnumber=6109224&tag=1](http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=6109224&tag=1)
- **“Using Compiler Directives for Accelerating CFD Applications on GPUs,”** H. Jin, M. Kellogg, and P. Mehrotra, 8<sup>th</sup> International Workshop on OpenMP, June 11-13, 2012, Rome, Italy.
- **“Performance Evaluation of Amazon EC2 for NASA HPC Applications,”** P. Mehrotra, J. Djomehri, S. Heistand, R. Hood, H. Jin, A. Lazanoff, S. Saini, and R. Biswas, 3<sup>rd</sup> Workshop on Scientific Cloud Computing (Science Cloud 2012), June 18, 2012, Delft, The Netherlands.
- **“An Application-Based Performance Evaluation of NASA’s Nebula Cloud Computing Platform,”** S. Saini, S. Heistand, H. Jin, J. Chang, R. Hood, P. Mehrotra (Session Chair), R. Biswas, HPCC 2012, June 25-27, 2012, Liverpool, UK.

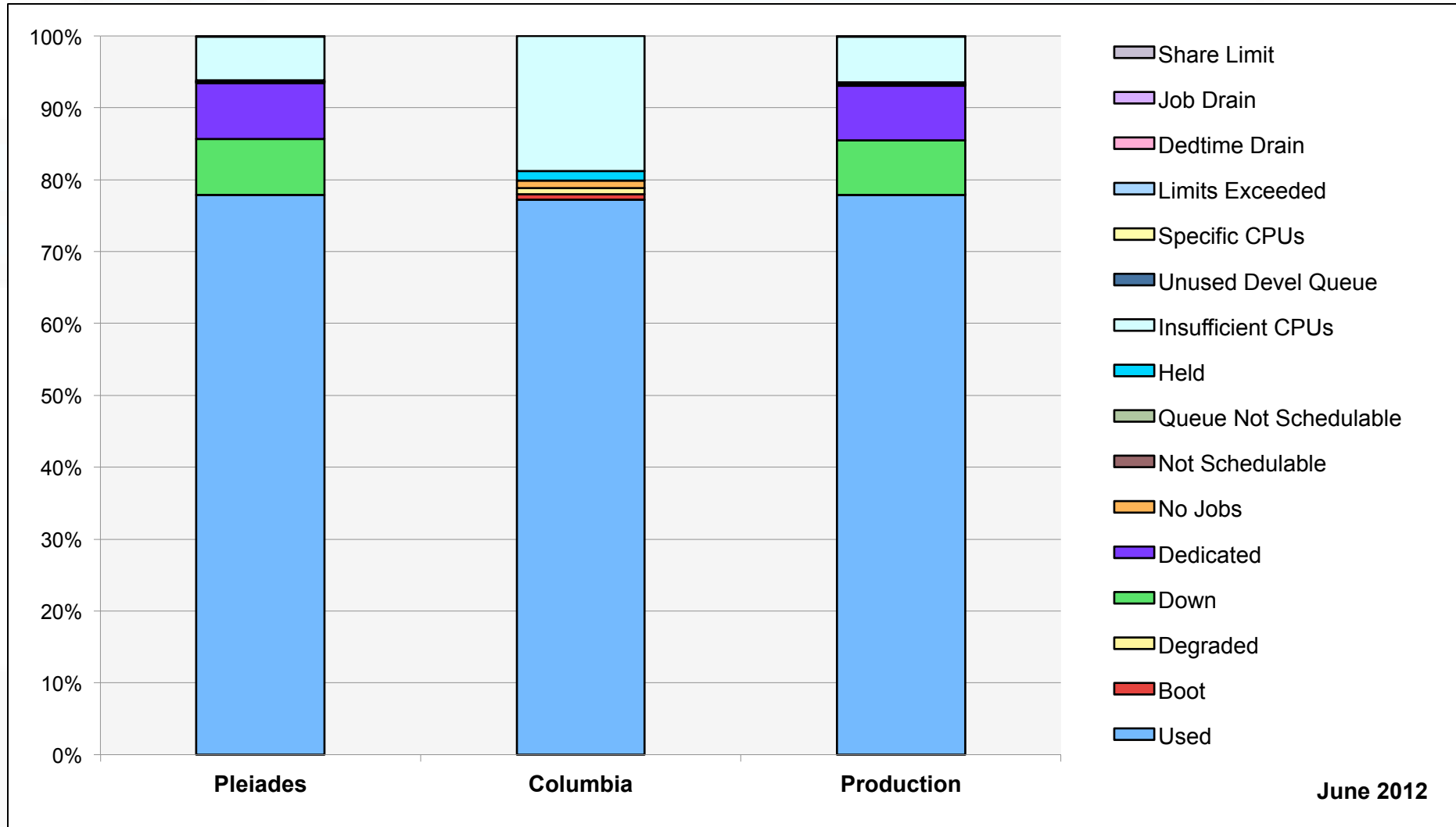
*\*HECC provided supercomputing resources and services in support of this work.*



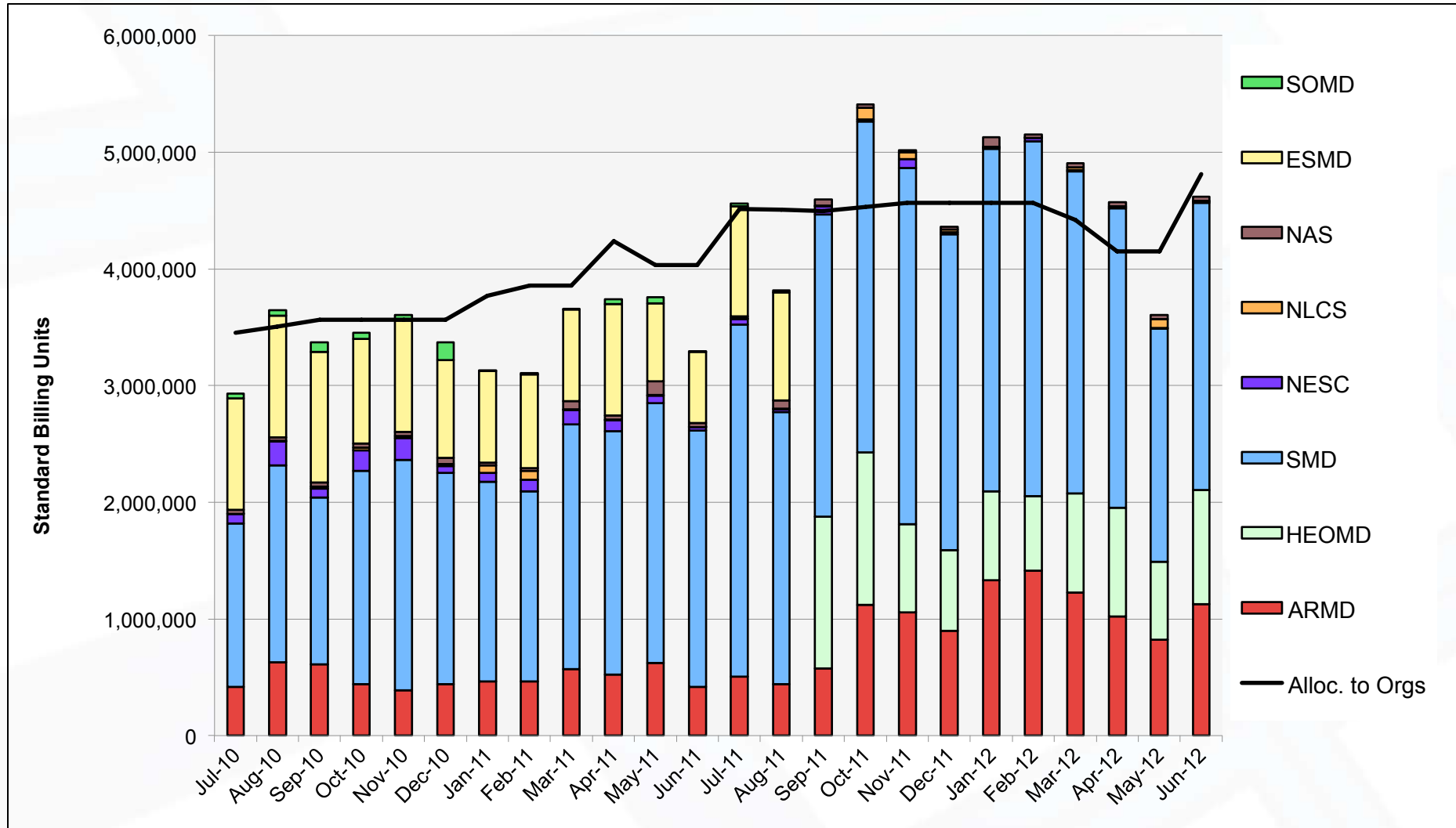
- **NASA'S Pleiades Supercomputer Gets A Little More Oomph**, *official NASA press release*, June 19, 2012 – This announcement of the recent system expansion was picked up by numerous media outlets including *HPCwire*, was covered on KLIV radio (San Jose), and generated a request from NBC TV to feature Pleiades in a segment of the local “Bay Area Proud” series.  
[http://www.nasa.gov/home/hqnews/2012/jun/HQ\\_12\\_206\\_Pleiades\\_Supercomputer.html](http://www.nasa.gov/home/hqnews/2012/jun/HQ_12_206_Pleiades_Supercomputer.html)
- **NASA Upgrades Pleiades Supercomputer**, *InformationWeek Government*, June 21, 2012  
Feature story covering the Pleiades expansion and related preparation work.  
<http://www.informationweek.com/news/government/enterprise-architecture/240002451>
- **Are Cloud Environments Ready for NASA HPC Applications?** HECC user webinar, May 31, 2012 – This webinar presented the results of a study comparing the performance of two cloud environments, Amazon's AWS and SGI's Cyclone, to that of NASA's Pleiades supercomputer to determine the suitability of cloud computing for HPC applications.  
[http://www.nas.nasa.gov/hecc/support/past\\_webinars.html](http://www.nas.nasa.gov/hecc/support/past_webinars.html)



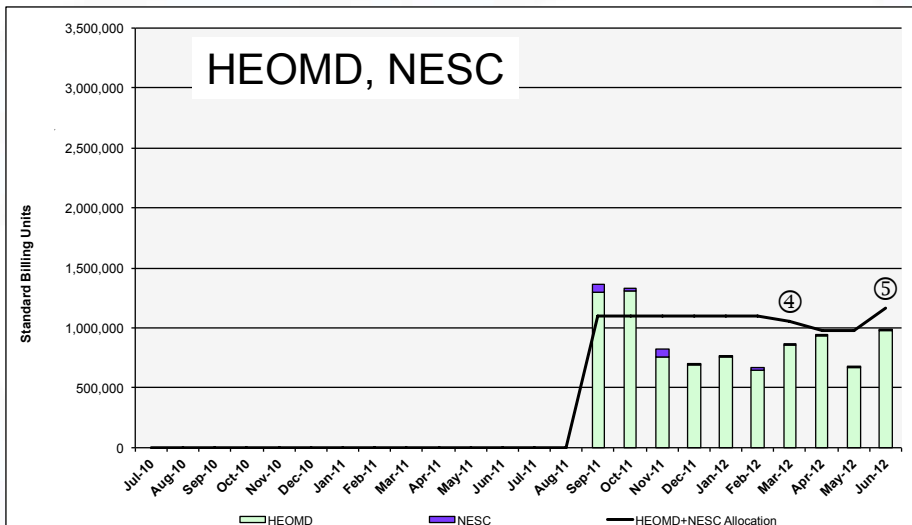
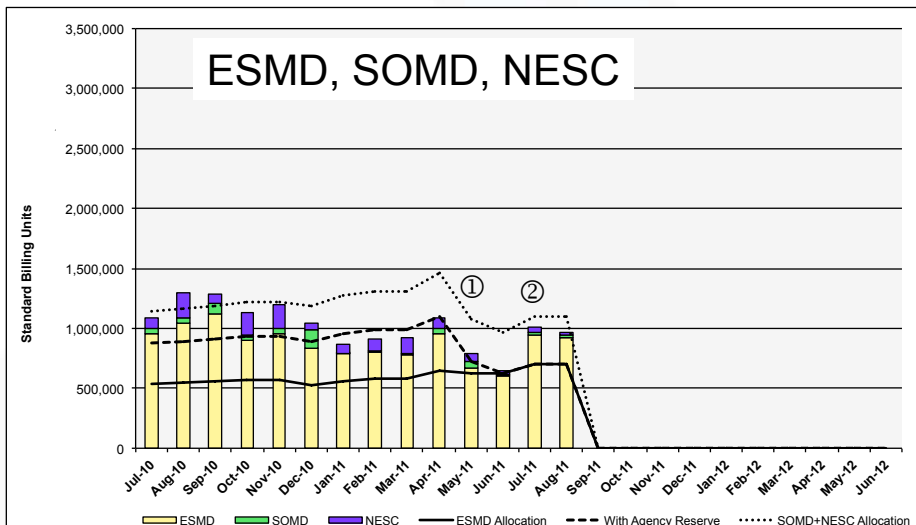
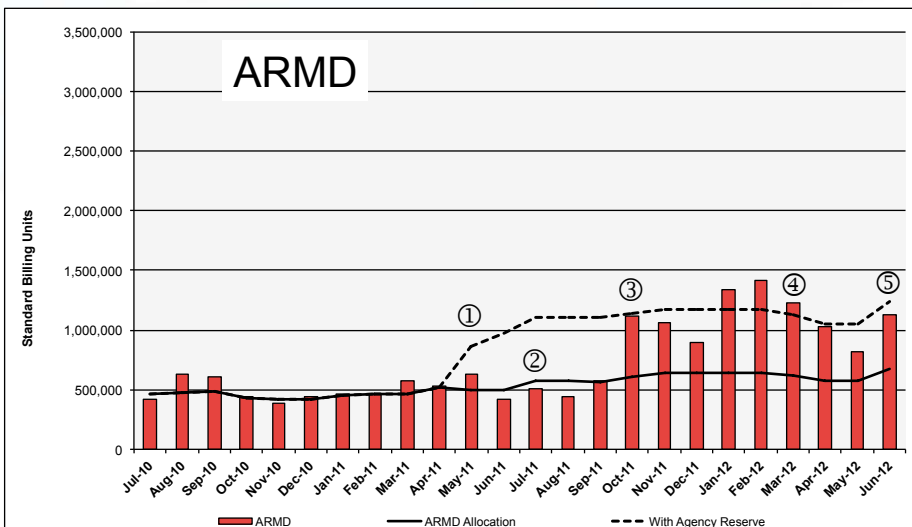
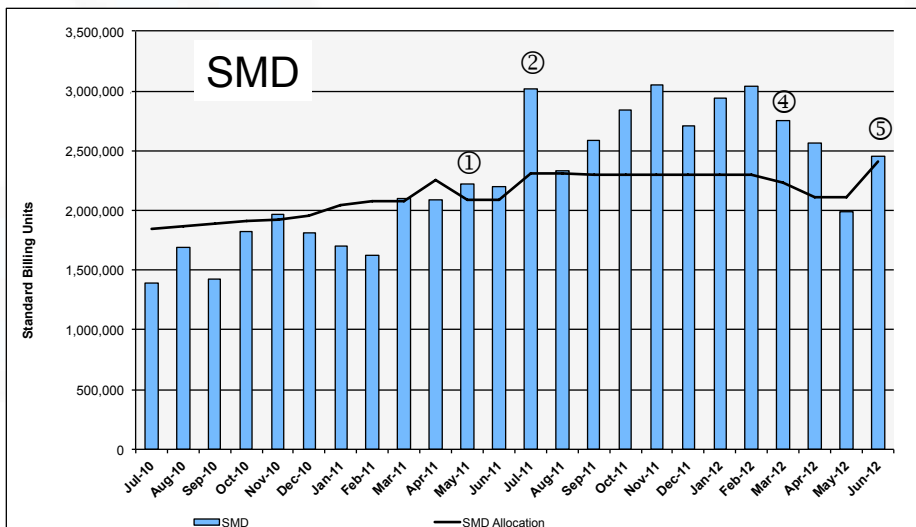
# HECC Utilization



# HECC Utilization Normalized to 30-Day Month



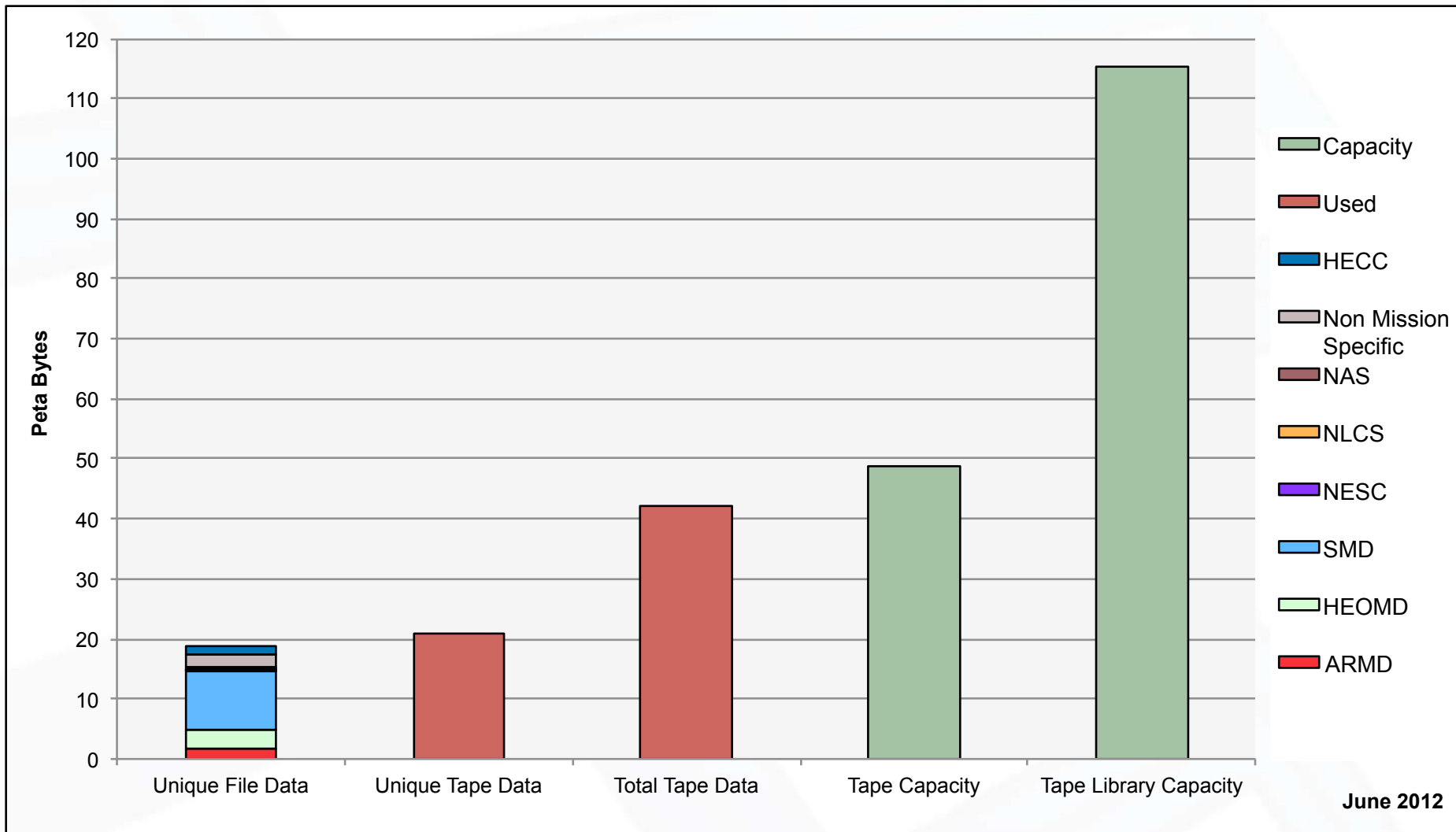
# HECC Utilization Normalized to 30-Day Month



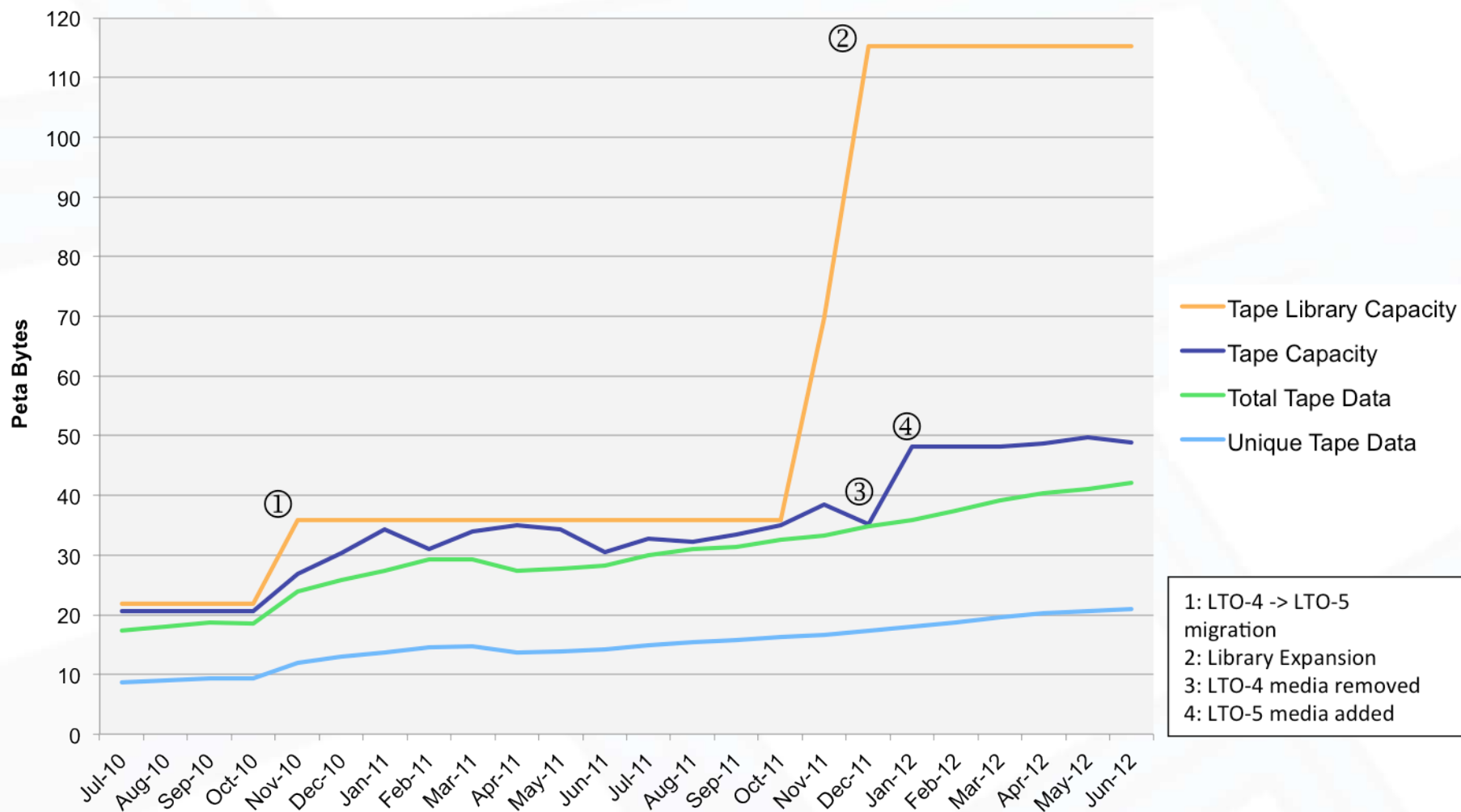
- ① Allocation to orgs. decreased to 75%, Agency reserve shifted to ARMD ② 14 Westmere racks added  
 ③ 2 ARMD Westmere racks added ④ 28 Harpertown racks removed ⑤ 24 Sandy Bridge racks added



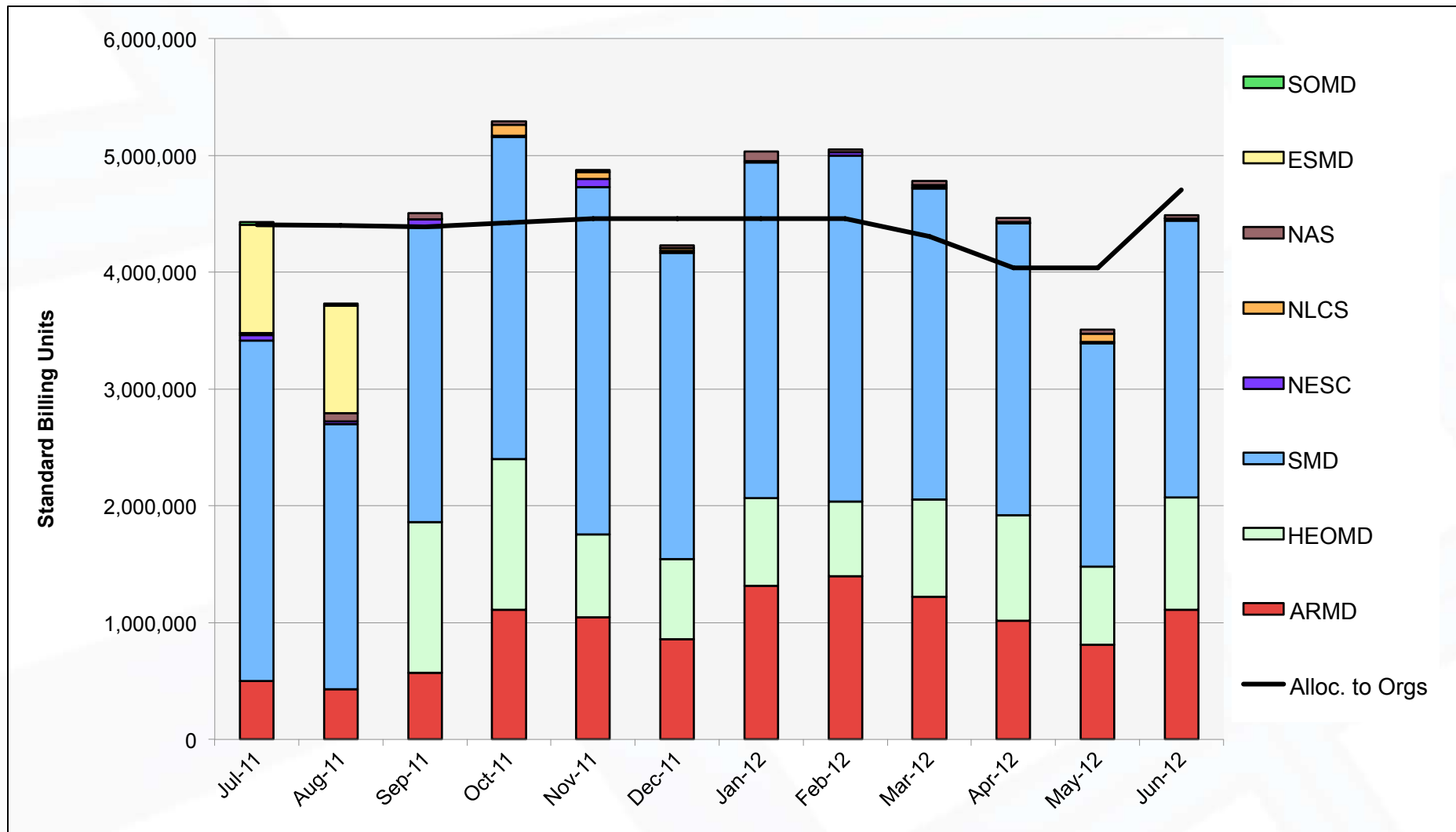
# Tape Archive Status



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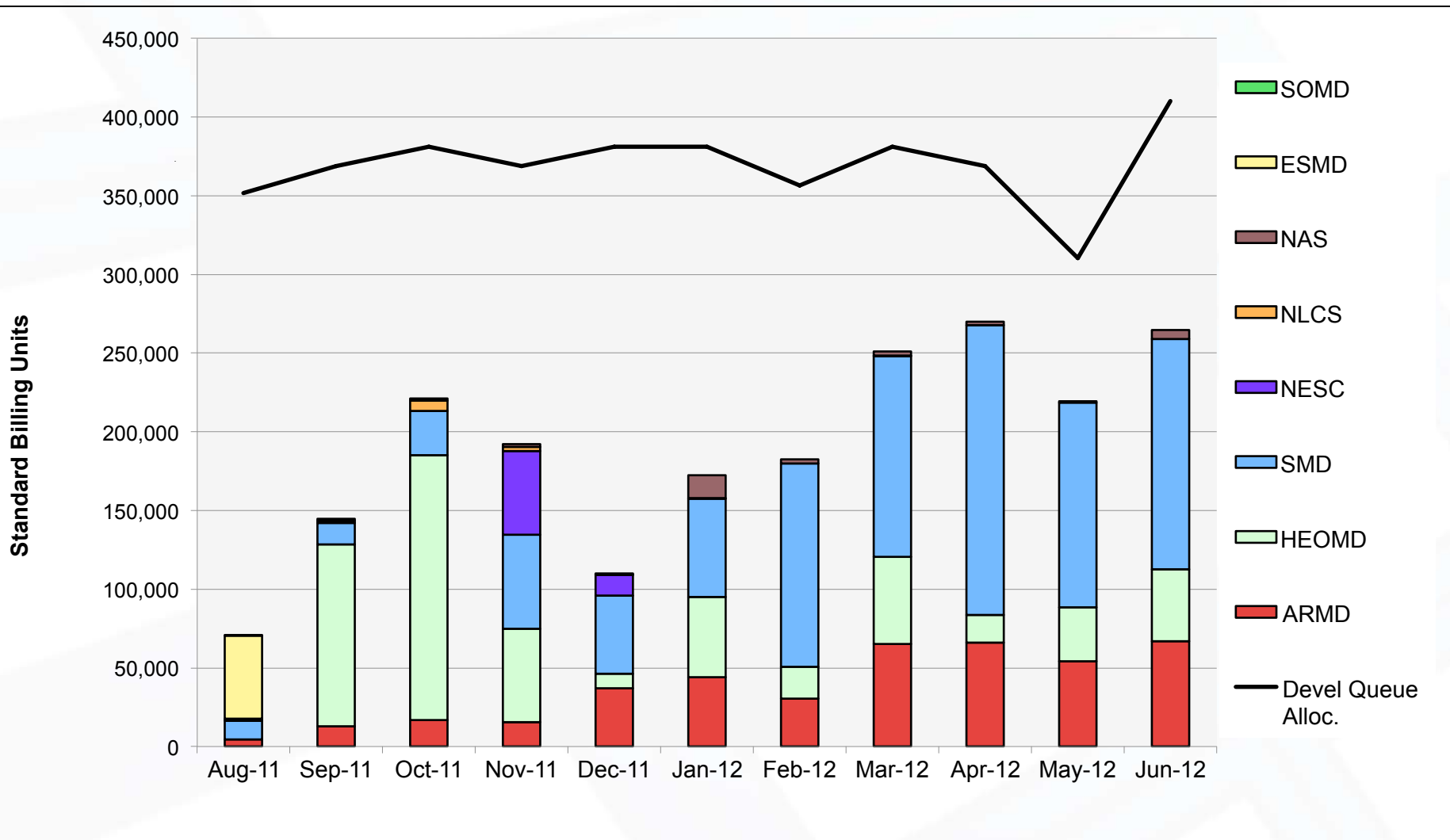


# Pleiades: SBUs Reported, Normalized to 30-Day Month

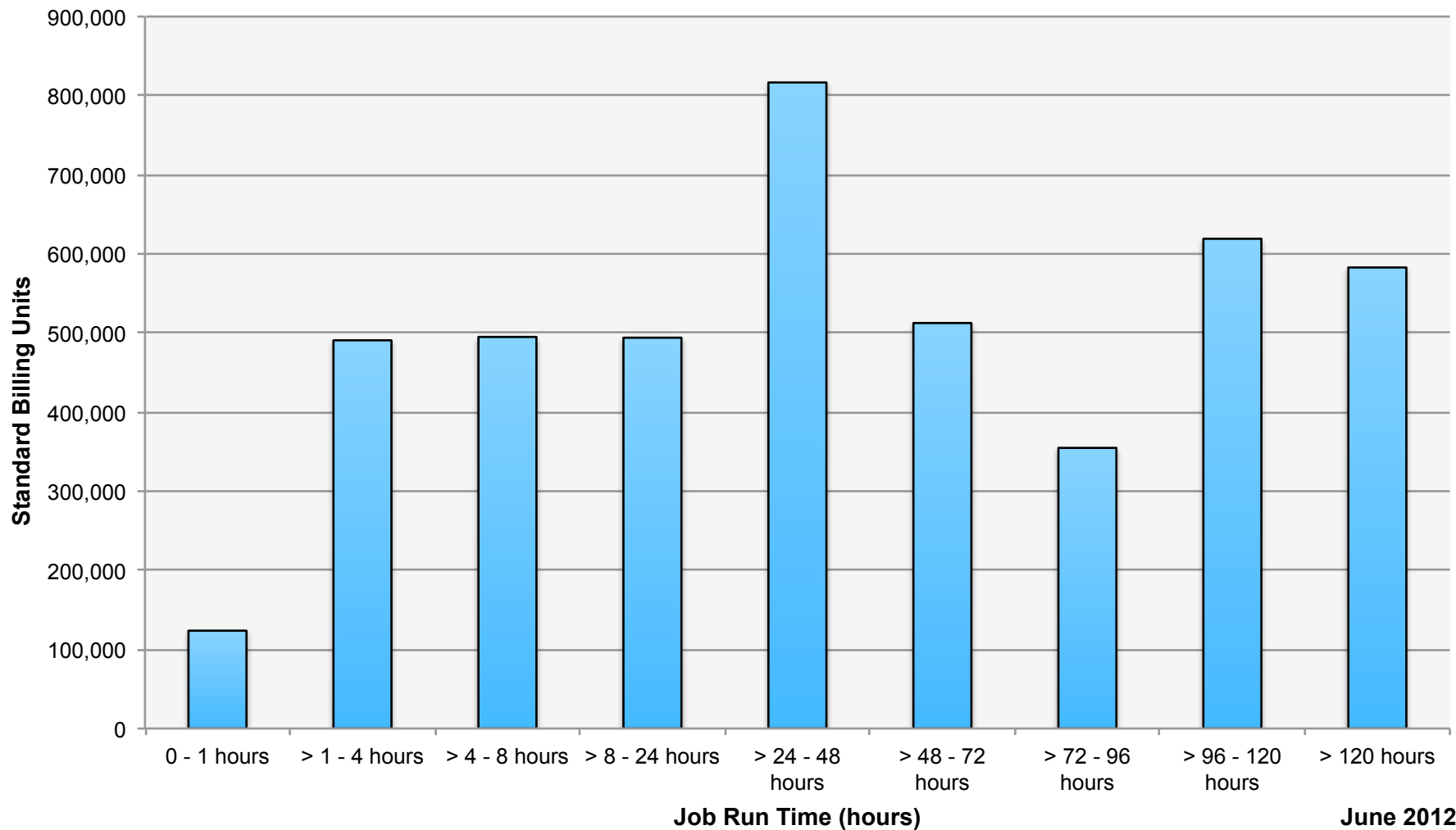




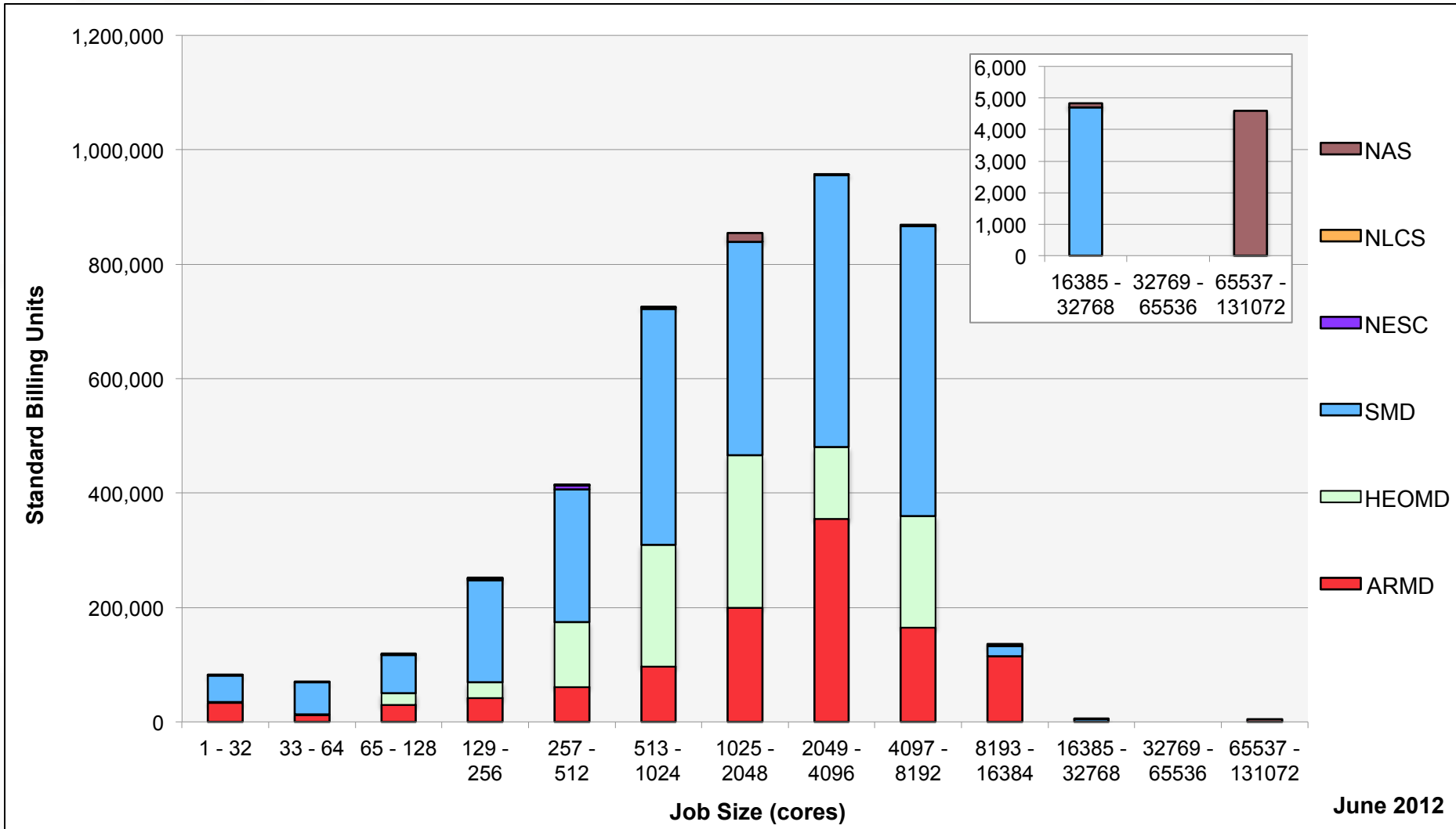
# Pleiades: Devel Queue Utilization



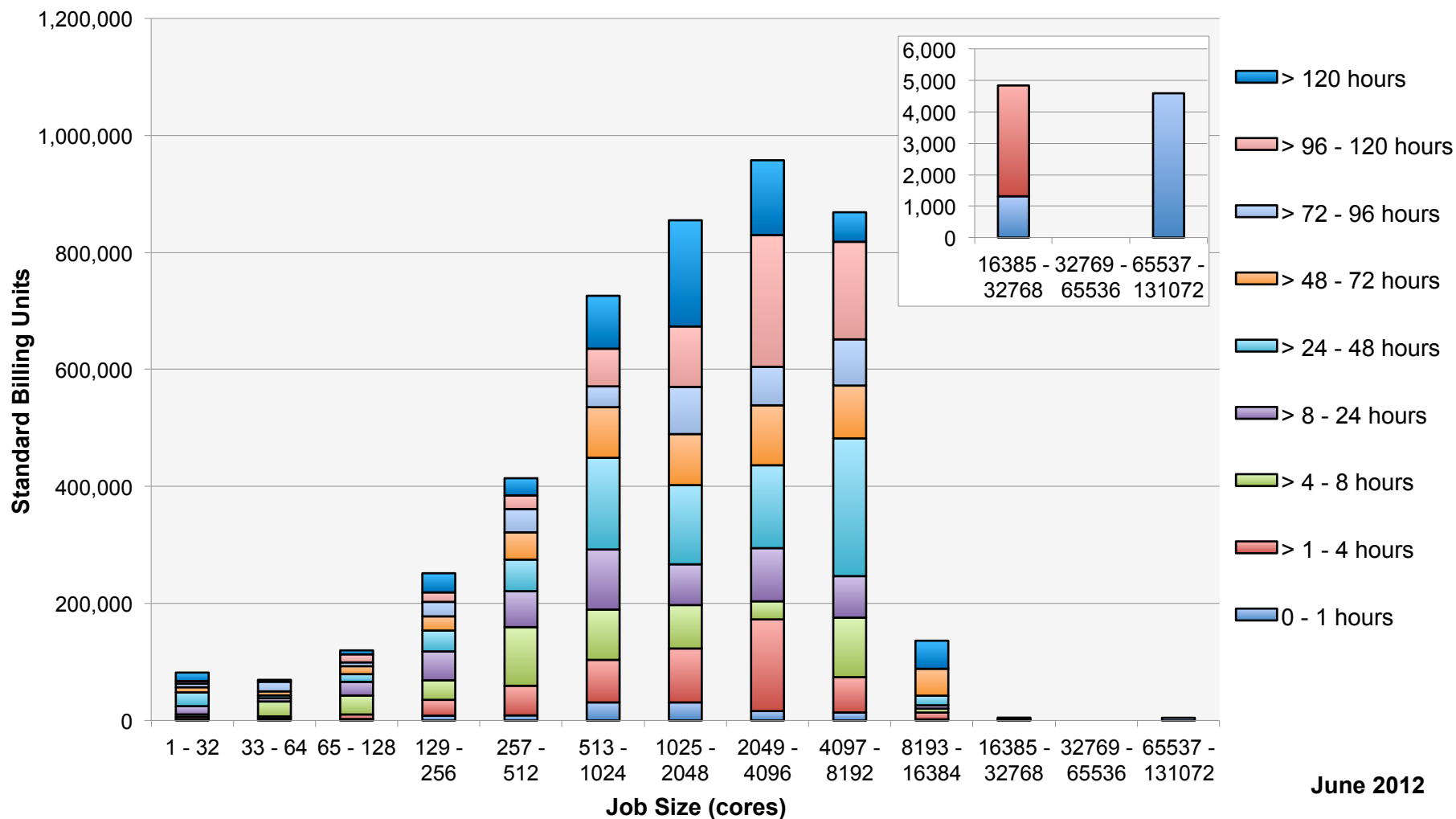
# Pleiades: Monthly SBUs by Run Time



# Pleiades: Monthly Utilization by Size and Mission

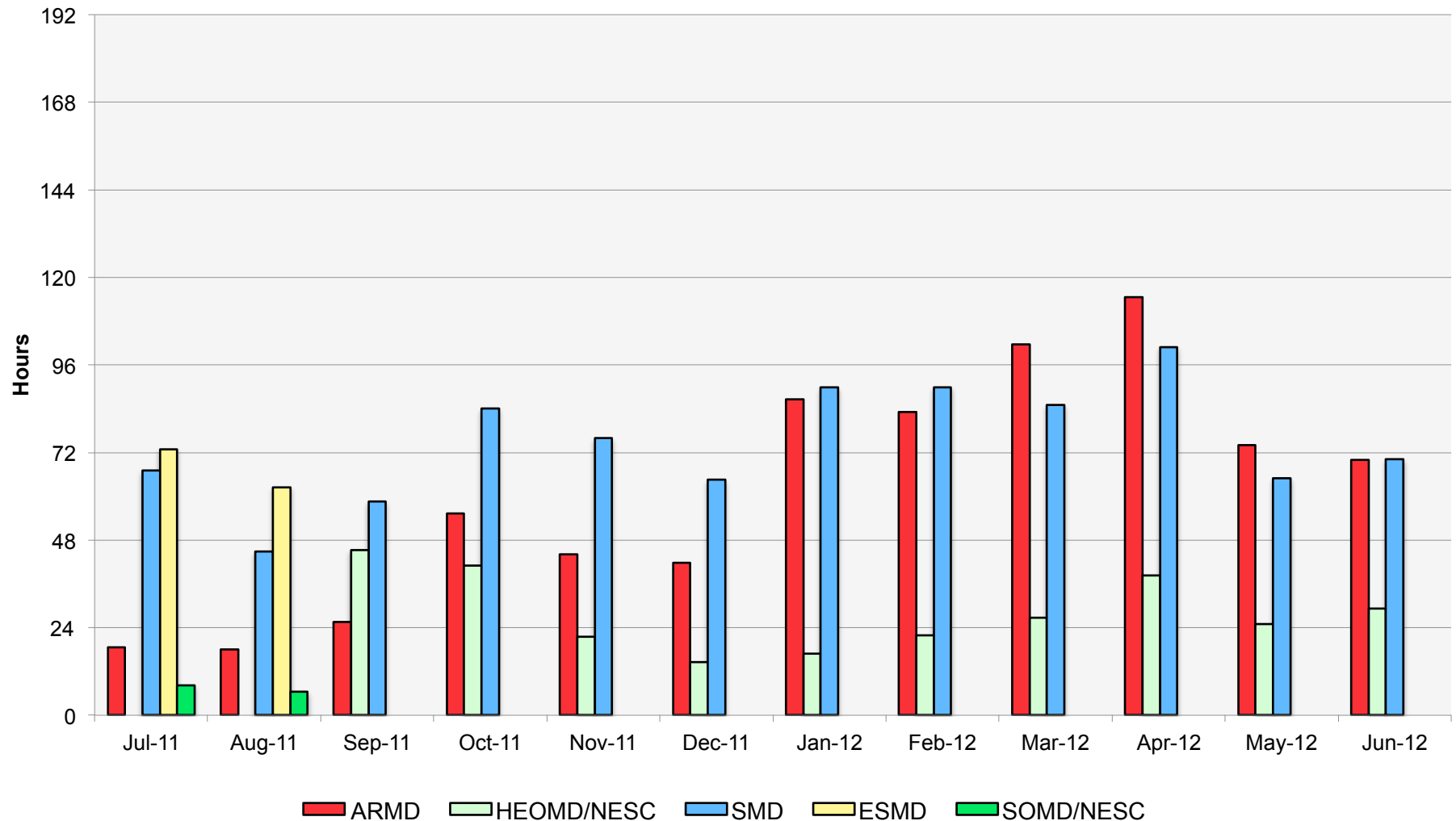


# Pleiades: Monthly Utilization by Size and Length

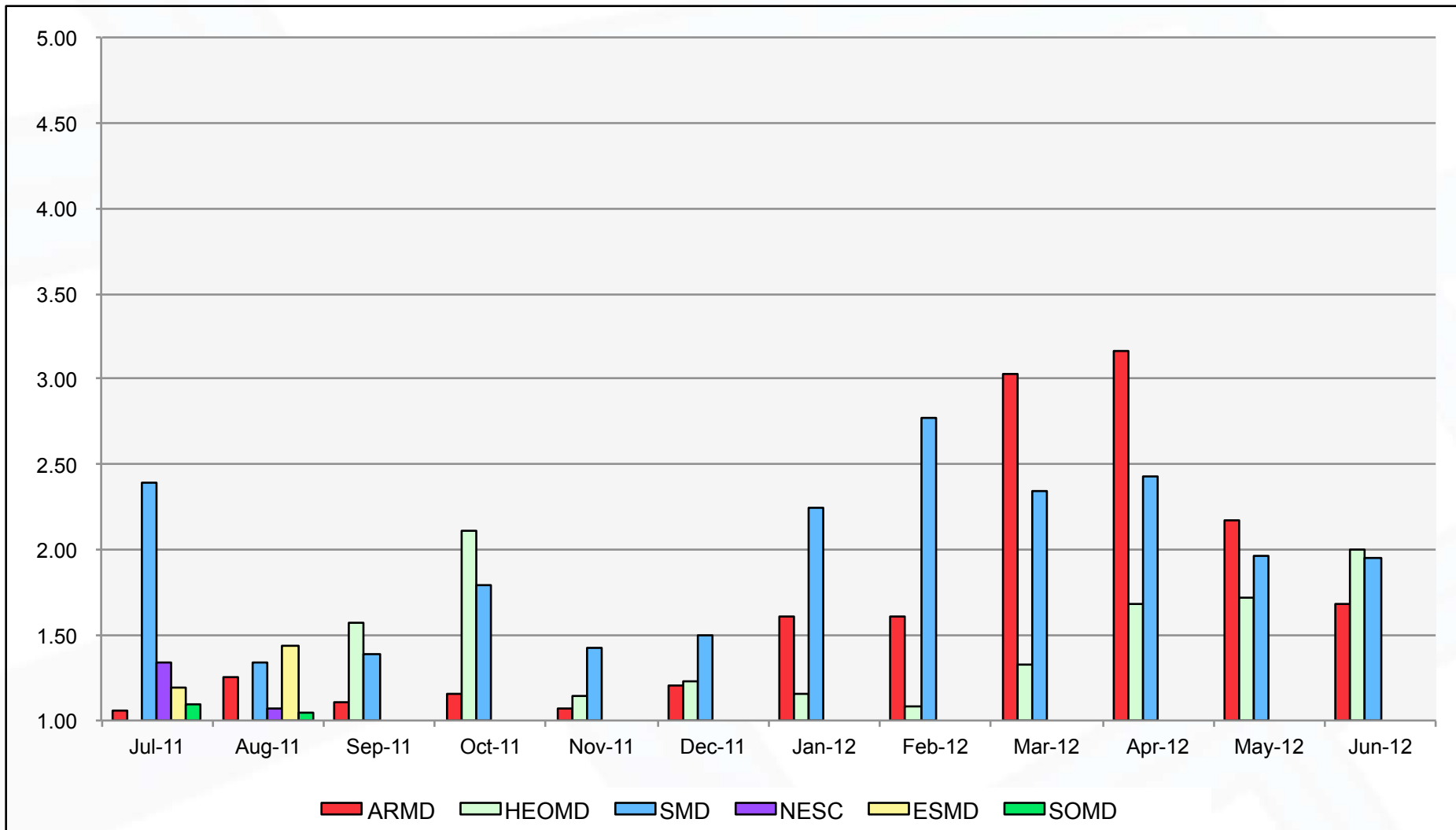




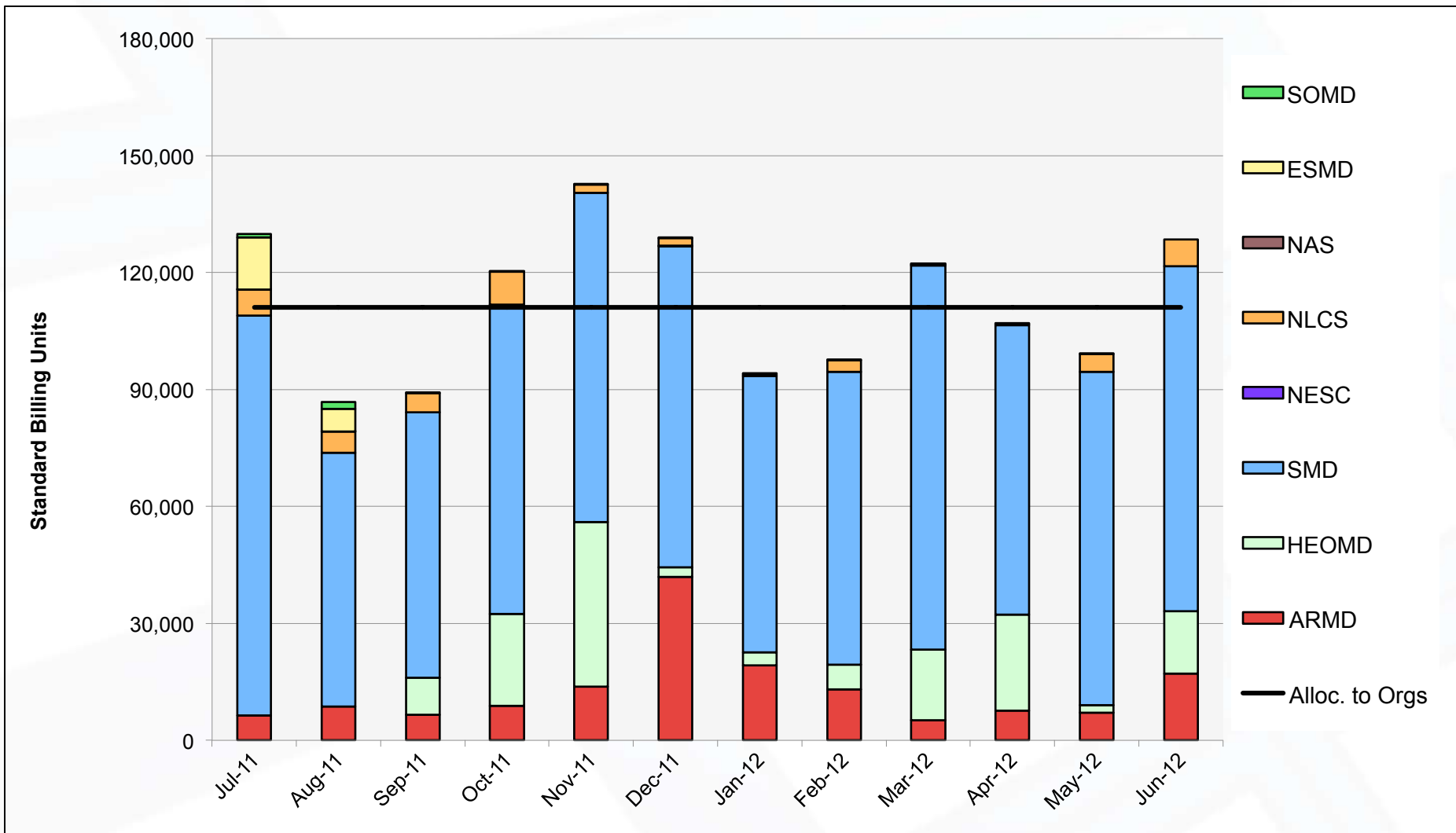
# Pleiades: Average Time to Clear All Jobs



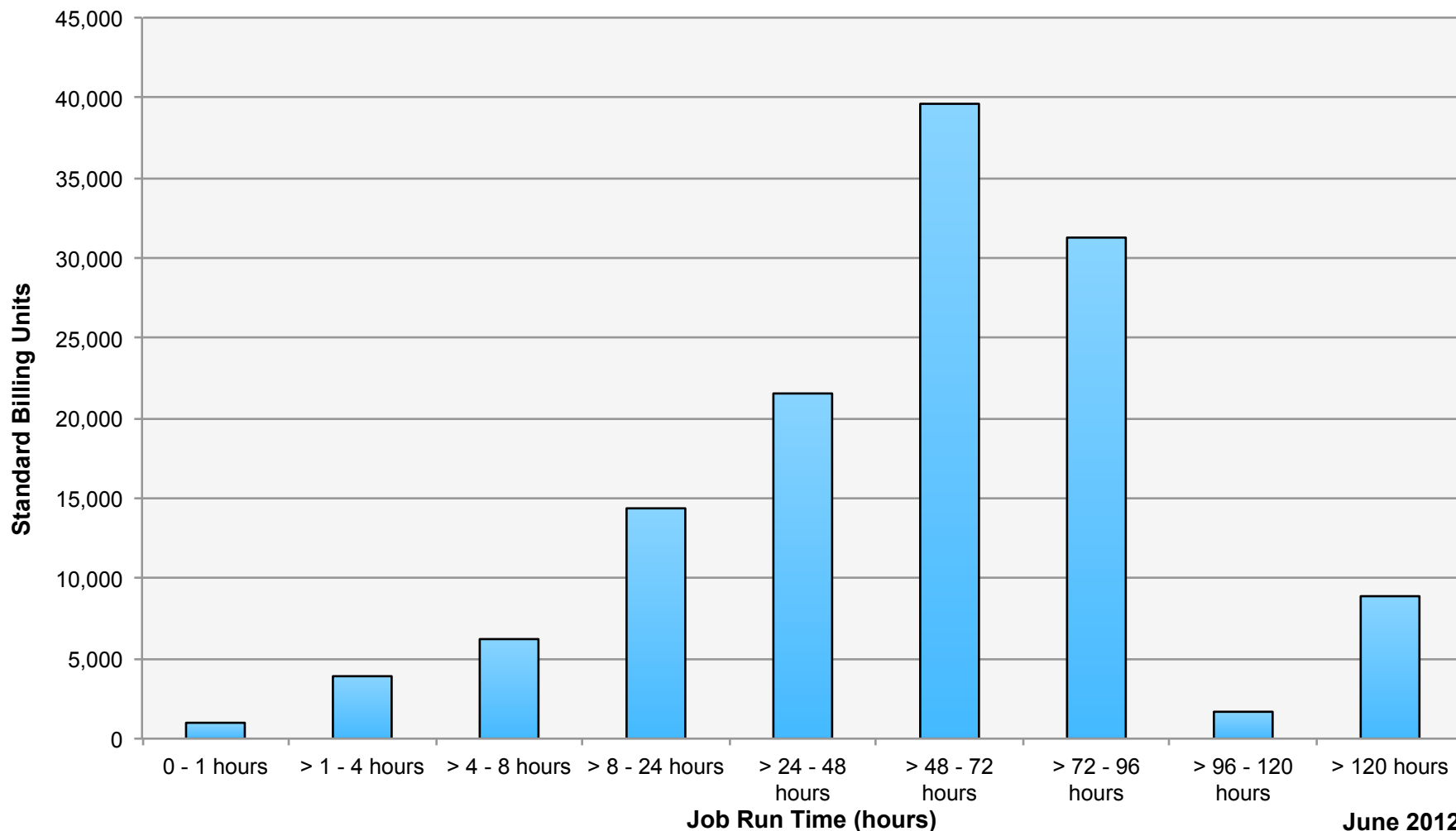
# Pleiades: Average Expansion Factor



# Columbia: SBUs Reported, Normalized to 30-Day Month

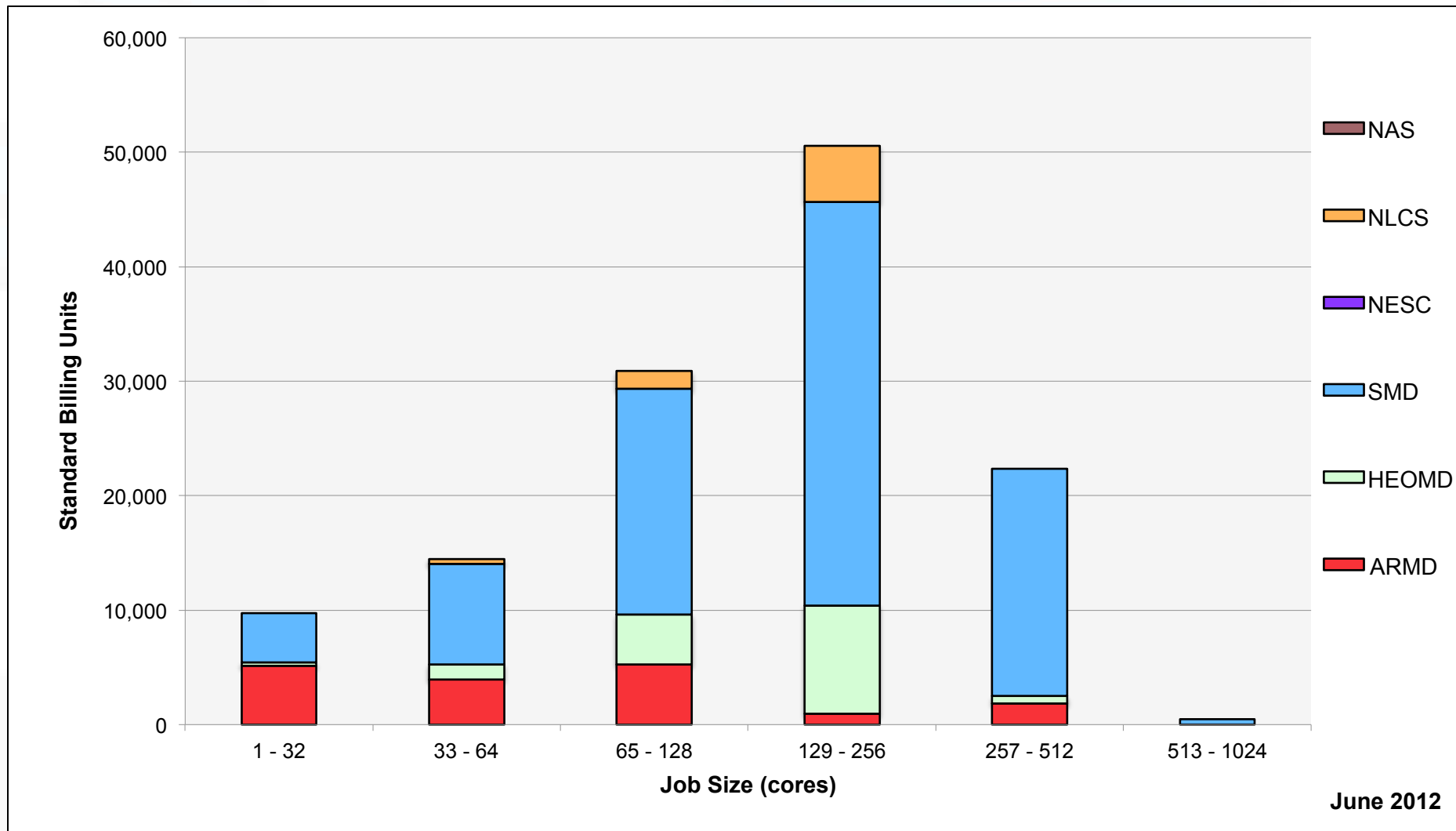


# Columbia: Monthly SBUs by Run Time

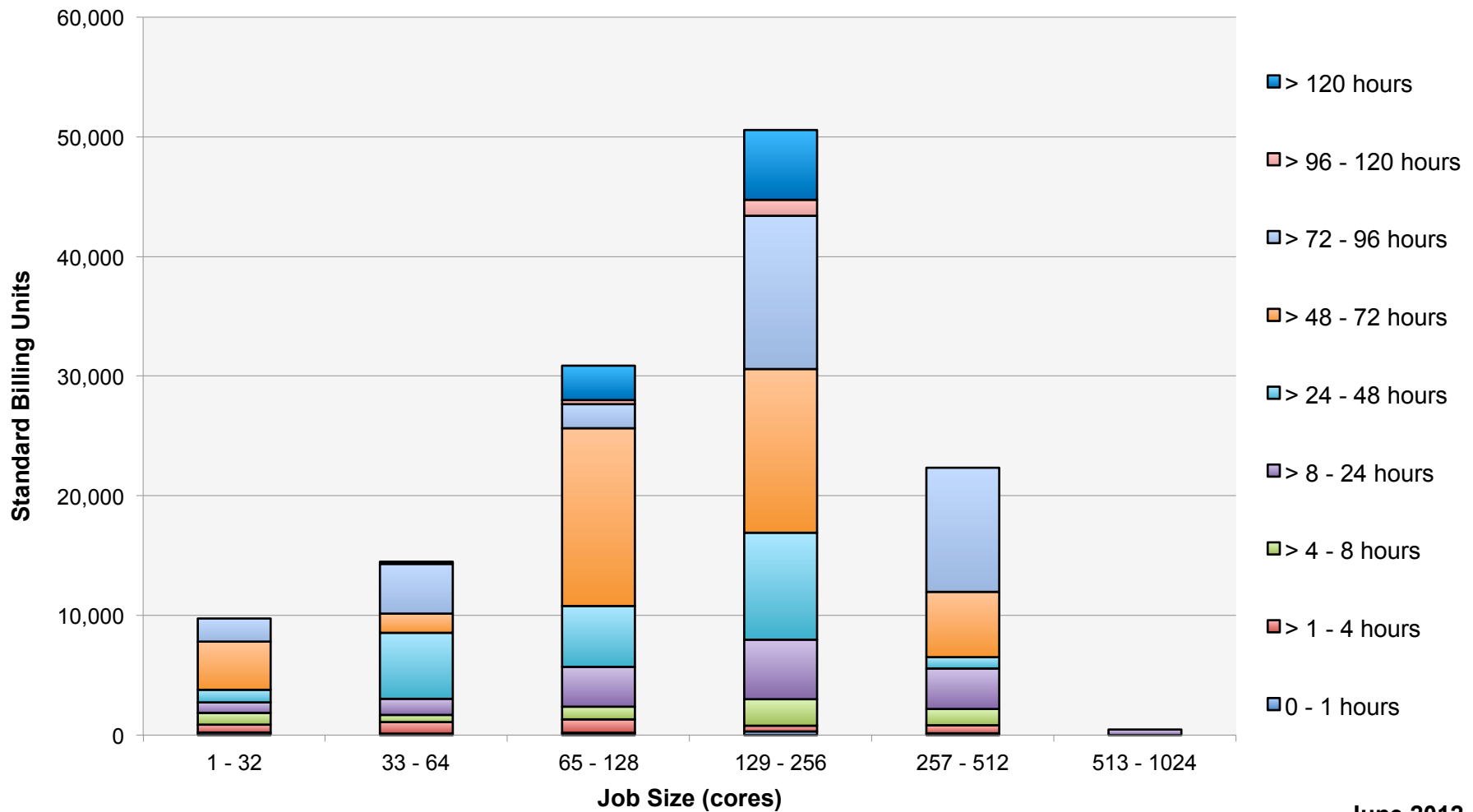




# Columbia: Monthly Utilization by Size and Mission

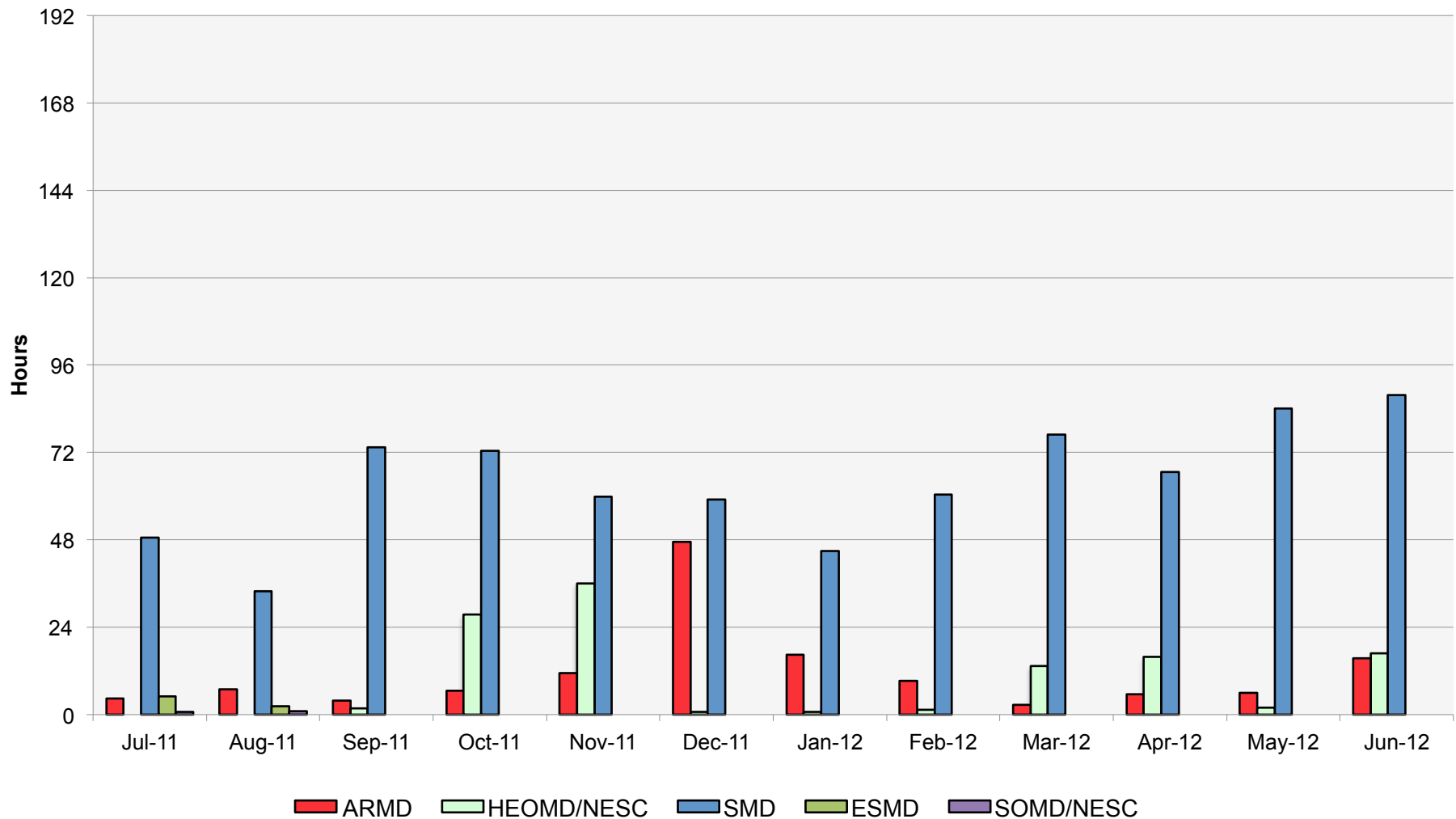


# Columbia: Monthly Utilization by Size and Length



June 2012

# Columbia: Average Time to Clear All Jobs



# Columbia: Average Expansion Factor

